

On the failure of subadditivity of the Wigner-Yanase entropy

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Abstract

It was recently shown by Hansen that the Wigner-Yanase entropy is, for general states of quantum systems, not subadditive with respect to decomposition into two subsystems, although this property is known to hold for pure states. We investigate the question whether the weaker property of subadditivity for pure states with respect to decomposition into more than two subsystems holds. This property would have interesting applications in quantum chemistry. We show, however, that it does not hold in general, and provide a counterexample.

In 1963, Wigner and Yanase [4] introduced the entropy-like quantity

$$S^{\text{WY}}(\rho, K) = \frac{1}{2} \text{Tr} [\rho^{1/2}, K]^2 = \text{Tr} \rho^{1/2} K \rho^{1/2} K - \text{Tr} \rho K^2 \quad (1)$$

for density matrices ρ of quantum systems, with K some fixed self-adjoint operator. They showed that S^{WY} is concave in ρ [4, 5] and, for pure states, subadditive with respect to decomposition of the quantum system into two subsystems. More precisely, if $|\psi\rangle$ is a normalized vector in the tensor product of two Hilbert spaces, $\mathcal{H}_1 \otimes \mathcal{H}_2$, and K_1 and K_2 are self-adjoint operators on \mathcal{H}_1 and \mathcal{H}_2 , respectively, then

$$S^{\text{WY}}(|\psi\rangle\langle\psi|, K_1 \otimes \mathbb{1} + \mathbb{1} \otimes K_2) \leq S^{\text{WY}}(\rho_1, K_1) + S^{\text{WY}}(\rho_2, K_2), \quad (2)$$

where $\rho_1 = \text{Tr}_{\mathcal{H}_2} |\psi\rangle\langle\psi|$ and $\rho_2 = \text{Tr}_{\mathcal{H}_1} |\psi\rangle\langle\psi|$ denote the reduced states of the subsystems. Recently, it was shown by Hansen [2] that this subadditivity *fails* for general mixed states.

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This leaves open the question whether the Wigner-Yanase entropy is sub-additive for pure states with respect to decompositions into *more* than 2 subsystems. If true, this property would have interesting consequences concerning density matrix functionals used in quantum chemistry, as will be explained below. We shall show, however, that this property does *not* hold, in general.

Let $\rho = |\psi\rangle\langle\psi|$ be a pure state on a tensor product of N Hilbert spaces, $\mathcal{H} = \bigotimes_{i=1}^N \mathcal{H}_i$, and let K_i be self-adjoint operators on \mathcal{H}_i . For simplicity we use the same symbol for the operators on \mathcal{H} which act as the identity on the remaining factors. Subadditivity of S^{WY} would mean that

$$\begin{aligned} -S^{\text{WY}}(|\psi\rangle\langle\psi|, \sum_i K_i) &= \left\langle \psi \left| (\sum_i K_i)^2 \right| \psi \right\rangle - \langle \psi | \sum_i K_i | \psi \rangle^2 \\ &\geq \sum_i \left(\text{Tr}_{\mathcal{H}_i} \rho_i K_i^2 - \text{Tr}_{\mathcal{H}_i} \rho_i^{1/2} K_i \rho_i^{1/2} K_i \right), \end{aligned} \quad (3)$$

where ρ_i is the reduced density matrix of $|\psi\rangle\langle\psi|$ on \mathcal{H}_i .

Assume now that all the \mathcal{H}_i are equal to the same \mathcal{H}_1 , say, and that also all the K_i are equal, i.e., K_i acts as K on the i 'th factor for some fixed operator K on \mathcal{H}_1 . Ineq. (3) together with concavity of S^{WY} would thus imply that

$$\left\langle \psi \left| (\sum_i K_i)^2 \right| \psi \right\rangle - \langle \psi | \sum_i K_i | \psi \rangle^2 \geq \text{Tr}_{\mathcal{H}_1} \gamma K^2 - \text{Tr}_{\mathcal{H}_1} \gamma^{1/2} K \gamma^{1/2} K, \quad (4)$$

or

$$\left\langle \psi \left| \sum_{i \neq j} K_i K_j \right| \psi \right\rangle \geq (\text{Tr}_{\mathcal{H}_1} \gamma K)^2 - \text{Tr}_{\mathcal{H}_1} \gamma^{1/2} K \gamma^{1/2} K, \quad (5)$$

where $\gamma = \sum_i \rho_i$ denotes the one-particle density matrix of $|\psi\rangle\langle\psi|$. This represents a *correlation inequality*, bounding from below two-particle terms in terms of one-particle terms only.

As explained in [1], the validity of (4) for continuous quantum systems in the case where K is the characteristic function of a ball of arbitrary size and location would imply that the ground state energies of Coulomb systems like atoms and molecules could be bounded from below by a density-matrix functional introduced by Müller [3]. For $N = 2$ this follows from the result in [4].

In the following, we shall show that, in general, (4) fails to hold for $N = 3$, and hence for all $N \geq 3$. We choose the simplest nontrivial three-particle Hilbert space, $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$, and pick a basis $\{|\uparrow\rangle, |\downarrow\rangle\}$ in \mathbb{C}^2 . We choose $K = |\uparrow\rangle\langle\uparrow|$, and¹

$$\begin{aligned} \psi(\uparrow, \uparrow, \uparrow) &= \frac{2}{\sqrt{55}} \\ \psi(\uparrow, \uparrow, \downarrow) &= \psi(\uparrow, \downarrow, \uparrow) = \psi(\downarrow, \uparrow, \uparrow) = \frac{4}{\sqrt{55}} \\ \psi(\uparrow, \downarrow, \downarrow) &= \psi(\downarrow, \uparrow, \downarrow) = \psi(\downarrow, \downarrow, \uparrow) = \frac{1}{\sqrt{55}} \\ \psi(\downarrow, \downarrow, \downarrow) &= 0. \end{aligned} \quad (6)$$

¹This particular counterexample was found with the aid of the computer algebra software *Mathematica*.

Then

$$\begin{aligned}
\langle \psi | \psi \rangle &= \frac{1}{55} (2^2 + 3 * 4^2 + 3 * 1) = 1 \\
\langle \psi | \sum_i K_i | \psi \rangle &= \frac{1}{55} (3 * 2^2 + 2 * 3 * 4^2 + 1 * 3 * 1) = \frac{111}{55} \\
\langle \psi | (\sum_i K_i)^2 | \psi \rangle &= \frac{1}{55} (3^2 * 2^2 + 2^2 * 3 * 4^2 + 1 * 3 * 1) = \frac{231}{55}
\end{aligned} \tag{7}$$

and hence the left side of Ineq. (4) equals

$$\frac{231}{55} - \left(\frac{111}{55} \right)^2 = \frac{384}{3025} \approx 0.126942. \tag{8}$$

The one-particle density matrix γ is given by the 2×2 -matrix

$$\gamma = \frac{3}{55} \begin{pmatrix} 37 & 16 \\ 16 & 18 \end{pmatrix} \tag{9}$$

whose square root equals

$$\gamma^{1/2} \approx \sqrt{\frac{3}{55}} \begin{pmatrix} 5.85827 & 1.63729 \\ 1.63729 & 3.91399 \end{pmatrix}. \tag{10}$$

Hence the right side of (4) is

$$\frac{3}{55} (37 - (5.85827)^2) \approx 0.146221 > 0.126942. \tag{11}$$

This shows that Ineq. (4) fails in general for $N > 2$, and hence the Wigner-Yanase entropy is not subadditive with respect to the decomposition of pure states into more than 2 subsystems.

We note that the same counterexample can also be constructed for continuous quantum systems, where K equals the characteristic functions of some measurable set B . One simply takes B and Ω to be two disjoint sets, each with volume one, and sets

$$\psi(x_1, x_2, x_3) = \frac{1}{\sqrt{55}} \begin{cases} 2 & \text{if all 3 particles are in } B \\ 4 & \text{if 2 particles are in } B \text{ and 1 in } \Omega \\ 1 & \text{if 1 particle is in } B \text{ and 2 in } \Omega \\ 0 & \text{otherwise.} \end{cases} \tag{12}$$

This leads to the same counterexample as above.

Similarly, one can construct a counterexample for fermionic (i.e., antisymmetric) wavefunctions which, after all, is the case of interest in [1]. Simply take (x, y) as the coordinates of one particle, choose the wave function to be the product of (12) for the x variables and a Slater-determinant for the y variables, which is non-zero only if all the y 's are in some set Λ . If K denotes multiplication by the characteristic function of $B \times \Lambda$, this leads to the same counterexample as before.

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